Class	M.Sc. Chemistry (Previuos)
Semester/Year	I Year
Subject & Subject Code	Chemistry - MCHEM20Y101
Paper	INORGANIC CHEMISTRY Paper- I
Max. Marks	60 (ETE) + 40 (IA) =100

Credit			Total Credits
L	T	P	4
3	1	0	

Course Objectives:

On completion of the course, students are able to:

To learn about bonding in polyacids, inorganic polymers, formation, factors that affect stability of complexing stereo isomerism of inorganic complexes and crystal field theory and its limitations.

Course Outcome:

At the end of the course, learners will be able to:

1. To know the structure and bonding in molecules / ions and predict the structure of molecules / ions.
2. To learn the periodic properties of the different groups of compounds focusing on production methods and application of selected elements and compounds.
3. To know the different definitions of acids / bases and predict the reactions between acids and bases.
4. To learn the selected crystal structures and to explain what kind of parameters that affects the crystal structure of a compound.
5. To be able to use Crystal Field Theory to understand the magnetic properties (and in simple terms the colour) of coordination compounds.
6. To be able to describe the stability of metal complexes by the use of formation constants and to calculate thermodynamic parameters from them.

Student Learning Outcomes (SLO):

Students will:

1. Students should be able to explain atomic structure based on quantum mechanics and explain periodic properties of the atoms.
2. Students should be able to explain selected crystal structures explain what kind of parameters that affect the crystal structure of a compound and perform calculations of the lattice enthalpy of ionic compounds.
3. Students should be able to explain the periodic properties of the different groups of compounds focusing on production methods and application of selected elements and compounds.
4. Students should be able to explain the band structure of solids and determine the electrical properties.
5. Students should be able to explaining the theory of the determination of the electron structure of d-metal complexes and explain the properties of these complexes.
6. Students should be able to explain the structure and bonding in molecules and predict the structure of molecules.

Unit	Syllabus	Periods
UNIT - I	**Stereochemistry and Bonding in Main Group Compounds** VSEPRT, Walsh diagram (tri-andpenta-atomic molecules), $d\pi$-$p\pi$ bonds, Bent rule and energetics of hybridization, some simple reactions of covalently bonded molecules. **Metal-Ligand Equilibriaum Solution** Step wise and over all formation constants and their interaction, trends in step wise constant, factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand. Chelate effect and its thermodynamic origin, determination of binary formation constants by pH-metry and spectrophotometry.	12
UNIT - II	**Reaction Mechanism of Transition Metal Complexes** Energy profile of a reaction, reactivity of metal complex, inert and labile complexes, kinetic application of valence bond and crystal field theories, kinetics of octahedral substitution, acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, direct and indirect evidences in favour of conjugate mechanism, anation reactions, reactions without metal ligand bond cleavage. Substitution reaction sin square planar complexes, the trans effect, mechanism of the substitution reaction. Redox reaction, electron transfer reactions, mechanism of one electron transfer reactions, outer sphere type reactions, cross reactions and Marcus-Hush theory, inner sphere type reactions.	12
UNIT - III	**Metal-Ligand bonding** Limitation of crystal field theory, molecular orbital theory,octahedral, tetrahedral and square planar complexes, π-bonding and molecular orbital theory.	12
UNIT - IV	**Electronic Spectra and Magnetic Properties of Transition Metal Complexes** Spectroscopic ground states, correlation.Orgel and Tanabe-Sugano diagrams for transition metal complexes (d1-d9 states), calculations of D α, β and β parameters, charge transfer spectra, spectroscopic method of assignmetnt of absolute configuration in optically active metal chelates and their stereochemical in formation, anomalous magnetic moments, magnetic exchange coupling and spin cross over.	12
UNIT - V	**Metal π- Complexes** Metal carboynl, structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation, important reactions of metal carbonyls; preparation, bonding structure and important reaction of transition metal nitrosyl, dinitrogen and dioxgen complexes; tertiary phosphineas ligand. **Metal Clusters** Higher boranes, carboranes, metalloboranes and metallocarboranes. Metal carbonyl and halide clusters,compounds with metal multiple bonds.	12

REFERENCE BOOKS –

1 Advanced Inorganic Chemistry, F. A. Cotton and Wilkinson, John Wiley.
2 Inorganic Chemistry, J. E. Huhey, Harpes & Row.
3 Chemistry of the Elements, N. N. Greenwood and A. Earnshow, Pergamon.
4 Inorganic Electronic Spectroscopy, A. B. P. Lever, Elsevier.
5 Magnetic chemistry, R.1. Carlin, Springer Verlag.
6 Comprehensive Coordiantion Chemistry eds.,G. Wilkinson, R. D. Gillars and J. A. Mc Cleverty, Pergamon.

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         Nodhi

Class	M.Sc. Chemistry (Previuos)
Semester/Year	I Year
Subject & Subject Code	Chemistry - MCHEM20Y102
Paper	ORGANIC CHEMISTRY Paper- II
Max. Marks	60 (ETE) + 40 (IA) =100

Credit			Total Credits
L	T	P	4
3	1	0	

Course Objectives:
On completion of the course, students are able to:
To learn about optical activity of asymmetric and dissymmetric molecules. Basic idea about aliphatic nucleophilic substitution reactions, aromaticity, aromatic nucleophilic and electrophilic substitution reactions

Course Outcome:
At the end of the course, learners will be able to:
1. To learn the concept stereochemistry and its importance.
2. To know what is aliphatic nucleophilic substitution.
3. To understand the various types of aliphatic nucleophilic substitution.
4. To learn what is aromatic substitution reaction.
5. To familiarize the various types of aromatic substitution reaction and their Mechanism.
6. To learn the concept aromaticity.
7. To understand the various types of aromaticity.
8. To learn the stereochemistry substitution and aromaticity.
9. To learn familiar name reactions.
10. To identify the stereochemical notation.

Student Learning Outcomes (SLO):
Students will:
1. Able to recognize either molecule is aromatic,non-aromatic or antiaromatic.
2. Able to describe mechanism of different aliphatic nucleophillic substitution reactions.
3. Able to draw potential energy diagrams.
4. Able to assign R and S to given molecules.
5. Able to do itnerconversion of Fischer to Newmann,Newmann to Sawhorse and vice versa.

Unit	Syllabus	Periods
UNIT - I	**Nature of Bonding in Organic Molecules** Delocalized chemical bonding-conjugation, cross conjugation, resonance hyperconjugation, bonding in fullerenes, tautomerism. Aromaticity in benzenoid and non-benzenoid compounds, alternate and non-alternate hydrocarbons. Huckel's rule, energy level of π- molecular orbitals, annulenes, anti-aromaticity, ψ aromaticity, homo-aromaticity, PMO approach. Bonds weaker than covalent-addition compounds, crown ether complexes and cryptands, inclusion compounds, catenanes and rotaxanes. **Stereo chemisty** Conformational analysis of cycloalkanes, decalins, effect of conformation on reactivity, conformation of sugars, strain due to unavoidable crowding Elements of symmetry, chirality, molecules with more than one chiral center, threo and erythroisomers, methods of resolution, optical purity, enantiotopic and diastereotopic atoms, groups and faces, stereospecific and stereo selective synthesis, Asymmetric synthesis. Optical activity in the absence of chiral carbon (biphenyls, allenes and spirane chirality due to helical shape. Stereochemistry of the compounds containing nitrogen, sulphur and phosphorus.	12
UNIT - II	**Reaction Mechanism: Structure and Reactivity** Type of mechanisms, types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle. Potential energy diagrams, transition states and intermediates, methods of determining mechanisms, isotopes effects Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes and nitrenes. Effect of structure on reactivity, resonance and field effects, steric effect, quantitative treatment. The Hammett equation and linear free energy relationship, subsistent and reaction constants, Taft equation. **Aliphatic Nucleophilic Substitution** The S_N^2, S_N^1 mixed S_N^1 and S_N^2 and SET mechanisms. The neighbouring group mechanism, neighbouring group participation by π and σ bonds, anchimeric assistance. Classical and non classical carbocations, phenonium ions, norbornyl systems, common carbocation rearrangements. Application of NMR spectroscopy in the detection of carbocations. The S_N^1 mechanism. Nucleophilic substitution at an allylic, aliphatic trigonal and a vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, phase transfer catalysis and ultrasound, ambident nucleophile, regioselectivity.	12
UNIT - III	**Aromatic Electrophilic Substitution** The areniumion mechanism, orientation and reactivity, energy profile diagrams. The ortho/para ratio, ipso attack, orientation in other ring systems. Quantitative treatment of reactivity in substrates and electrophiles. Diazonium coupling, Vilsmeir reactiion, Gatterman-Koch reaction. **Aromatic Nucleophilic Substitution** The S_N ArS_N^1, benzyne and S_{RN} mechanism, Reactivity effect of substrate structure, leaving group and attacking nucleophile. The Von Richte, Sommelet Hauser, and Smiles rearrangements. **Free Radical Reactions** Types of free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate, neighbouring group assistance. Reactivity for aliphatic and aromatic substrates at a bridgehead. Reactivity in the attacking radicals. The effect of solvents on reactivity. Allylic halogenation (NBS), oxidation of aldehydes to carboyxlic acids, auto- oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts, Sandmeyer reaction. Free radical rearrangement. Hunsdiecker reaction.	12

UNIT - IV	**Addition to Carbon-Carbon Multiple Bonds** Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regio-and chemo selectivity, orientation and reactivity. Addition to cyclopropane ring. Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Hydroboration, Michael reaction, Sharpless asymmetric epoxidation. **Addition to Carbon-Hetero Multiple bonds** Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acid esters and nitriles. Addition of Grignard reagents, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds. Witting reaction. Mechanism of condensation reactions involving enolates-Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions. Hydrolysis of esters and amides, ammonolysis of esters.	12	
UNIT - V	**Elimination Reactions** The E2, E1 and E1 cB mechanisms and their spectrum. Orientation of the double bond. Reactivity effects of substrate structures, attacking base, the leaving group and the medium. Mechanism and orientation in pyrolytic elimination. **Pericyclic Reactions** Molecular orbital symmetry, Frontier orbitals of ethylene,1,3- butadiene,1,3,5 -hexatriene and allyl system. Classification of pericyclic reactions. Woodward-Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reactions-conrotatory and disrotatory motions, 4n 4n+2 and allyl systems. Cycloadditions and tarafacial and suprafacial additions, 4n and 4n+2 systems, 2+2 addition of ketenes, 1,3 dipolar cycloadditions and cheleotropic reactions. Sigmatropic rearrangements-suprafacial and antarafacial shifts of H, sigmatropic involving carbon moieties, 3,3- and 5,5 sigmatropic rearrangements. Claisen, Cope and azaope rearrangements. Fluxional tautomerism. Ene reaction.	12	

REFERENCE BOOKS –

1 Advanced Organic Chemistry: Reactions, Mechanism & Structure, Jerry March, J.Wiley.

2

3 A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.

4 Press.

5 Organic Chemistry, R. T. Morrison and R. N. Boyd, Prentice-Hall.

6 Modern Organic Reactions, H. O. House, Benjamin.

7 Principles of Organic Synthesis, R. O. C. Norman and J. M. Coxon, Blackie Academic & Profes

8 Reaction Mechanism in Organic Chemistry, S. M. Mukherji and S. P. Singh,Mc Millan.

9 Pericyclic Reactions, S. M. Mukherji, Mc Millan, India

10 Stereochemistry of Organic Compounds, D. Nasipuri, New Age International.

11 Stereochemisty of Organic Compounds, P. S. Kalsi, New Age International.

12 Pericyclic Reactions: Ameta, Sharma, Vardia, Vyas, Sadguru Publications.

Class	M.Sc. Chemistry (Previuos)
Semester/Year	I Year
Subject & Subject Code	Chemistry - MCHEM20Y103
Paper	PHYSICAL CHEMISTRY Paper- III
Max. Marks	60 (ETE) + 40 (IA) =100

Credit			Total Credits
L	T	P	
3	1	0	4

Course Objectives:
On completion of the course, students are able to:
1. To learn about the concept of phase and derivation of phase rule.
2. To understand the Phase diagram for one component system and for two completely miscible component systems.
3. To study eutectic systems and calculation of eutectic point.
4. To understand ClausiusClapeyron equation and its applications.
5. To study kinetics of reaction in solution and influence of pressure, ionic strength, solvent on reaction rates.

Course Outcome:
At the end of the course, learners will be able to:
1. Students will acquire a good knowledge on the chemical kinetics, unimolecular and bimolecular reactions, fast reactions, Catalysis, Surface chemical reactions and Photochemistry of atoms and molecules.
2. An introduction to the chemistry, preparation, structure and physical properties of inorganic nanoparticles. Students will learn about methods to synthesize inorganic nanoparticles, and learn to evaluate particle size and shape distributions.
3. At the end of the class, they will be able to predict the stability of nanoparticles in solution, and to understand the nucleation and growth of nanoparticles.
4. They will know how to analyze the size-dependent physical properties of nanoparticles, and they will know about the different techniques (electron microscopy, X-ray diffraction) to study nanoparticles. Students will also be aware of applications of nanoparticles in science and technology.
5. It is expected that students enrolled in this class have a basic understanding of physical chemistry.

Student Learning Outcomes (SLO):
Students will:
1. Understand the concept of Phase and Gibb's Phase rule.
2. Study Phase diagram for one component and two component systems and calculate eutectic point, congruent and incongruent melting points.
3. Describe Kinetics of reaction in solution and in catalytic reactions.
4. Calculate Michaelis's constant for enzyme-substrate binding by Lineweaver-Burk plot.
5. Understand the concept of distribution and thermodynamic probability.
6. Evaluate most probable distribution state for all type of statics i.e. for MaxwellBoltzmann, Fermi dirac and Bose –Einstein statistics.
7. Understand the concept of partition function, its physical significance and calculation of molar and atomic partition function.

Unit	Syllabus	Periods
UNIT - I	**Quantum Chemistry** **Introduction to Exact Quantum Mechanical Results** The Schrodinger equation and the postulates of quantum mechanics. Discussion of solutions of the Schrodinger equation to some model systesm viz. particle in a box, the harmonic oscillator, the rigid rotor, the hydrogen atom. **Approximate Methods** The variation theorem, linear variation principle. Perturbation theory (First order and nondegenerate). Applications ofvariation method and perturbation theory to the Helium atom. **Angular Momentum** Ordinary angular momentum, generalized angular momentum,eigenfunctions for angular momentum, eigenvalues of angular momentum, operator using ladder operators addition of angular momentum, spin, antisymmetry and Pauli's exclusion principle. **Molecular Orbital Theory** Huckel theory of conjugated systems bond and charge density calculations. Applications to ethylene,butadiene, cyclopropenyl radical cyclobutadiene etc. Introduction to extended Hckel theory.	12
UNIT - II	**Classical Thermodynamics** Brief resume of concepts of laws of thermodynamics,free energy, chemical potential and entropies. Partial molar free energy, partial molar volume and partial molar heat constant and their significance. Determinations of these quantities. Concept of fugacity and determination of fugacity. **Non-ideal systems:** Excess functions for non-ideal solutions. Activity and activity coefficient, Debye Huckel theory for activity coefficient of electrolytic solutions; determination of activity and activity coefficients ; ionic strength. Application of phase rule to three component systems; second order phase transitions. **Statistical Thermodynamics** Concept of distribution, thermodynamic probability and most probable distribution. Ensemble averaging, postulates of ensemble averaging. Canonical, grand canonical and microcanonical ensembles, corresponding distribution laws (using Lagrange's method of undetermined multipliers). Partition functions-translation, rotational, vibrational and electronic partition functions, Calculation of thermodynamic properties in terms of partition. Application of partition functions. **Heat capacity behaviour of solids-** Chemical equilibria and equilibrium constant in terms of partition functions, Fermi-Dirac statistics, distribution law and applications to metal. Bose-Einstein statistics, distribution law and application to helium. **Non-Equilibrium Thermodynamics** Thermodynamic criteria for non-equilibrium states, entropy production and entropy flow, entropy balance equations for different irreversible processes (e.g., heat flow, chemical reaction etc.) transformations of the generalized fluxes and forces, non equilibrium stationary states, phenomenological equations, microscopic reversibility and Onsager's reciprocity relations, electrokinetic phenomena, diffusion, electric conduction, irreversible thermodynamics for biological systems, coupled reactions.	12

UNIT - III	**Chemical Dynamics** Methods of determining rate laws, collision theory of reaction rates, steric factor, activated complex theory, Arrhenius equation and the activated complex theory; ionic reactions, kinetic salt effects, steady state kinetics, kinetic and thermodynamic control of reactions, treatment of unimolecular reactions. Dynamic chain (hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane), photochemical (hydrogen-bromine and hydrogen-chlorine reactions) and homogenous catalysis, kinetics of enzyme reactions, general features of fast reactions, study of fast reactions by flow method, relaxation method, flash photolysis and the nuclear magnetic resonance method, dynamics of unimolecular reactions (Lindemann Hinshelwood and Rice-Ramsperger-Kassel-Marcus (RRKM) theories of unimolecular reactions).	12
UNIT - IV	**Surface Chemistry** **Adsorption** Surface tension, capillary action, pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, estimation of surface area (BET equation), Surface films on liquids (Electro-kinetic phenomenon), catalytic activity at surfaces. **Micelles** Surface active agents, classification of surface active agents, micellization, hydrophobic interaction, critical micellar concentration (CMC), factors affecting the CMC of surfactants, counter ion binding to micelles, thermodynamics of micellization-phase separation and mass action models, solublization, micro emulsion, reverse micelles. **Macro molecules** Polymer definition, types of polymers, electrically conducting, fire resistant, liquid crystal polymers, kinetics of polymerization, mechanism of polymerization. Molecular mass, number and mass average molecular mass, molecular mass determination (Osmometry, viscometry, diffusion and light scattering methods), sedimentation, chain configuration of macro molecules, calculation of average dimension of various chain structures.	12
UNIT - V	**Electro chemistry of solutions:** Debye-Huckel-Onsager treatment and its extension, ionsolvent interactions. Debye-Hückel-Jerum mode. Thermodynamics of electrified interface equations. Derivation of electro capillarity, Lippmann equations (surfac eexcess), methods of determination. Structure of electrified interfaces. Guoy-Chapman, Stern, Grahmam Devanatham-Mottwatts, Tobin, Bockris, Devanathan models, Over potentials, exchange current density, derivation of Butler Volmer equation, Tafel plot. **Quantum aspects of charge transfer at electrodes-** Solution interfaces, quantization of charge transfer, tunneling. Semi conductor interfaces-theory of double layer at semiconductor, electrolyte solution interfaces, structure of double layer interfaces. Effect of light at semiconductor solution interface. **Electocatalysis**: Influence of various parameters. Hydrogen electrode. Bioelectro chemistry, threshold membrane phenomena, Nernst-Planck equation, hodges-Huxley equation; core conductor models, electro cardiography. Polarography theory, Ilkone equation; half wave potential and its significance. Introduction to corrosion, homogenous theory, forms of corrosion monitoring and prevention methods.	12

REFERENCE BOOKS –

1. Physical Chemistry, P.W. Atkins, ELBS.

2. Introductionto Quantum Chemistyry, A.K. Chandra, Tata Mc Graw Hill.

3. Quantum Chemistry, IraN. Levine, Prentice Hall.

4. Coulson's Valence, R. Mc Weeny, ELBS.

5. Chemical Kinetics. K.J. Laidler, Mc Graw- Hill.

6. Kinetics and Mechanism of Chemical Transformation J. Rajaraman and J. Kunacose, Mc Millan.

Class	M.Sc. Chemistry (Previuos)
Semester/Year	I Year
Subject & Subject Code	Chemistry - MCHEM20Y104
Paper	Group Theory, Spectroscopy and Diffraction Methods Paper- IV
Max. Marks	45 (ETE) + 30 (IA) =75

Credit			Total Credits
L	T	P	3
3	0	0	

Course Objectives:
On completion of the course, students are able to:
1. To introduce the concepts and importance of symmetry and group theory in solving chemical problems.
2. To impart knowledge of spectroscopic techniques for structural analysis of organic compounds.
3. To impart the knowledge of electronic, rotation, vibration. NMR, FTIR, ESR, spectroscopy and their applications.

Course Outcome:
At the end of the course, learners will be able to:
1. Concepts of symmetry and group theory in solving chemical structural problems.
2. Use of character tables and projection operator techniques.
3. Application of symmetry and group theory in spectroscopy.
4. Microwave, Infrared-Vibration-rotation Raman and infra-red Spectroscopy and their applications for chemical analysis
5. Electronic spectroscopy of different elements and simple molecules.
6. Nuclear Magnetic and Electron Spin Resonance Spectroscopy for organic compounds analysis, medical diagnostics.

Student Learning Outcomes (SLO):
Students will:
1. Describe the selection rule for infrared-active transitions.
2. Determine the vibrations for a triatomic molecule and identify whether they are infrared-active.
3. Determine whether the molecular vibrations of a triatomic molecule are Raman active.
4. Explain the difference between Stokes and anti-Stokes lines in a Raman spectrum.
3. Justify the difference in intensity between Stokes and anti-Stokes lines.
5. Draw the Stokes and anti-Stokes lines in a Raman spectrum of a compound when given the energies of the different transitions.
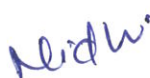6. Students will be able to Draw character table and point groups.

Unit	Syllabus	Periods
UNIT - I	**Symmetry and Group Theory in Chemistry** Symmetry elements and symmetry operation, definition of group, sub group, relation between or dersofafinite group all its sub group. Conjugacy relation and classes. Point symmetry group. Sch Ön flies symbols, representations of groups by matrices (representation for the C_n C_{nv}, C_{nh}, D_{nh}, etc. group to be worked out explicitly). Character of representation. The great orthogonality theorem (without proof) and its importance. Charactertables and their use; spectroscopy. **Unifying Principles** Electromagnetic radiation, interaction of electromagnetic radiation with matter absorption, emission, transmission, reflection, refraction, dispersion, polarisation and scattering. Uncertainity relation and natural line width and natural line broadening, transition probability, results of the time dependent per turbationtheory, transitionmoment, selection rules, intensity of spectral lines, Born-Oppen heimer approximation, rotational, vibrational and electronic energy levels.	9
UNIT - II	**Microwave Spectroscopy** Classification of molecules, rigid rotator model, effect of isotopic sub stitution on the transition frequencies, intensities,non-rigid rotor. Starkeffect, nuclear and electron spin interaction and effect of external field applications. **Vibrational Spectroscopy Infrared Spectroscopy** Review of linear harmonic oscillator, vibrational energies of diatomic molecules, zero point energy, force constant and bond strengths; anharmonicity, Morse potential energy diagram, vibration-rotation spectroscopy, P.Q.R. branches. Break down of Oppenheimer approximation; vibrations of polyatomic molecules. Selection rules, normal modes of vibration, group frequencies, overtones, hot bands, factors affecting the band positions and intensities, far IR region, metallig and vibrations, normal co-ordinate analysis. **Raman Spectroscopy** Classical and quantum theories of Raman effect. Pure rotational, vibrational and vibrational-rotational Raman spectra, selection rules, mutual exclusion principle, Resonance Raman Spectroscopy. Coherent Antistokes Raman Spectroscopy (CARS).	9
UNIT - III	**ElectronicSpectroscopy Atomic Spectroscopy** Energies of atomic orbitals, vector representation of momenta and vector coupling, spectra of hydrogen atom and alkali metal atoms. **Molecular Spectroscopy** Energy levels, molecular orbitals, vibronictran sitions, vibrational progressions and geometry of the excited states, Franck-Condon principle, electronic spectra of polyatomic molecules. Emission spectra; radiative and non- radiative decay, internal conversion, spectra of transition metal complexes, charge-transfer spectra. **Photoelectron Spectroscopy** Basic principles; photo-electric effect,ionization process, Koopman's theorem. Photoelectron spectra of simple molecules, ESCA, chemical in formation from ESCA. Auger electron spectroscopy-basic idea.	9

UNIT - IV	**Magnetic Resonance Spectroscopy Nuclear Magnetic Resonance Spectroscopy** Nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift and its measurements, factors, in fluencing chemical shift, deshielding, spin-spin interactions, factors in fluencing coupling constant "j" Classification (AVB, AMX, ABC, A2B2 etc.). spindecoupling; basic idea sab out in strument, NMR studies of nuclei other than proton-^{13}C, ^{19}F and ^{31}P. FT NMR, advantages of FTNMR, use of NMR in medical diagnostics. **Electron Spin Resonance Spectroscopy** Basic principles, zero field splitting and Kramer's degeneracy, factors affecting the 'g' value. Isotropic and anisotropic hyper fine coupling constants, spin hamiltonian, spin densities and Mc Connell relationship, measurement techniques, applications. **Nuclear Quadrupole Resonance spectroscopy** Quadrupole nuclei, quadrupole moments, electric field gradients, couplingconstant, splitting, applications.	9
UNIT - V	**Diffraction Methods** X-ray Diffraction Bragg condition, Miller indices, Laue Method, Bragg method, Debye Scherrer method of X-ray structural analysis of crystals, index reflections, identification of unit cell from systematic absences in diffraction pattern, Structure of simple lattices and X-ray in tensities, structure factor and its relation to intensity and electron density, phase problem. Description of the proced ureforan X-ray structure analysis, absolute configuration of molecules. **Electron Diffraction** Scattering intensity vs. scattering angle, Wierl equation, measurement technique, elucidation of structure of simple gas phase molecules. Low energy electron diffraction and structure of surfaces. **Neutron Diffraction** Scattering of neutrons by solids and liquids, magnetic scattering measurement techniques. Elucidation of structure of magnetically ordered unit cell.	9

REFERENCE BOOKS –

1. Modern Spectroscopy, J. M. Hollas, John Wiley.

2. Applied Electron Spectroscopy for chemical analysised. H. Windawi and F. L.Ho, Wiley Inter sc

3. NMR, NQR, EPR and Mössbauer Spectroscopy in Inorganic Chemistry, R. V.Parish, Ellis Harw

4. Physical Methodsin Chemistry, R. S. Drago,Saunders College.

5. Chemical Applications of Group Theory, F. A. Cotton.

6. Introduction to Molecular Spectroscopy, G. M. Barrow, Mc Graw Hill.

7. Basic Principles of Spectroscopy, R. Chang, Mc Graw Hill.

8. Theory and Application of U V Spectroscopy, H. H.Jaffe and M. Orchin, IBH-Oxford.

9. Introduction to Photoelectron Spectroscopy, P. K. Ghosh, John Wiley.

10. IntroductiontoMagneticResonance.Acarringtonand A.D.McLachalan,Harper&Row.

School of Basic and Applied Sciences

Class	M.Sc. Chemistry (Previuos)
Semester/Year	I Year
Subject & Subject Code	Chemistry - MCHEM20Y105
Paper	MATHEMATICS FOR CHEMISTS Paper- V (a1)
Max. Marks	15 (ETE) + 10 (IA) =25

Credit			Total Credits
L	T	P	
1	0	0	1

Course Objectives:
On completion of the course, students are able to:
The objective is to develop basic computing skills and application of quantitative and statistical operations required for biological studies and rationalization of experimental designs.

Course Outcome:
At the end of the course, learners will be able to:
Students will acquire mathematical concepts in continuous learning and connecting ideas like numerical analysis, calculus, coordinate geometry to other subjects and support learning through applications of mathematics.

Student Learning Outcomes (SLO):
Students will:
1. Having a clear understanding of the subject related concepts and of contemporary issues
2. Having computational thinking
3. Having Virtual Collaborating ability
4. Having problem solving ability- solving social issues and engineering problems
5. Having critical thinking and innovative skills

Unit	Syllabus	Periods
UNIT - I	**Vectors** Vectors, dot, cross and triple products etc. gradient, divergence and curl, Vector Calculus, Gauss'theorem, divergence theorem etc.	3
UNIT - II	**Matrix Algebra** Addition and multiplication; inverse, adjoint and transpose of matrices, special matrices (Symmetric, skew-symmetric, Hermitian, Skey-Harmitian, unit,diagonal, unitary etc.)and their properties. Matrix equations: Homogeneous, non-homogeneous linear equations and conditions for the solution, linear dependence and independence. Introduction to vector spaces,matrix eigen values and eigen vectors,diagonalization, determinants (examples from Hückel theory). Introduction to tensors; polarzability and magnetic susceptibility as examples.	3

UNIT - III	**Differential Calculus** Functions, continuity and differentiability, rules for differentiation, applications of differential calculus including maxima and minima (examples related to maximally populated rotational energy levels, Bohr's radius and most probable velocity from Maxwell's distribution etc.).exact and inexact differentials with their applications to thermodynamic properties. Integral calculus, basic rules for integration, integration by parts, partial fractions and substitution. Reduction formulae, applications of integral calculus. Functions of several variables,partial differentiation,coordinate transformations (e.g.cartesian to spherical polar) curve sketching.	3
UNIT - IV	**Elementary Differential equations** Variables-separable and exact first order differential equations, homogenous, exact and linear equations. Applications to chemical kinetics, secular equilibria, quantum chemistry etc. solution of differential equations by the power series method, Fourier series, solutions of harmonic oscillator and legend reequation etc., spherical harmonics, second order differential equation and their solutions.	3
UNIT - V	**Permutation and Probability** Permutations and combinations, probability and probability theorems, average, probability curves,root mean square and most probable errors, examples from the kinetic theory of gases etc., curve fitting (including least squares fit etc.) with a general polynomial fit.	3

REFERENCE BOOKS –

1 The Chemistry Mathematics Book, E. Steiner, Oxford University Press.
2 Mathematics for Chemistry, Doggett and Sucliffe, Longman.
3 Mathematical for Physical Chemistry: F. Daniels, Mc Graw Hill.
4 Chemical Mathematics D. M. Hirst, Longman.
5 Applied Mathematics for Physical Chemistery, J.R. Barrnte, Prentice Hall.
6 Basic Matchematics for Chemists,Tebbutt, Wiley.

Class	M.Sc. Chemistry (Previuos)
Semester/Year	I Year
Subject & Subject Code	Chemistry - MCHEM20Y106
Paper	BIOLOGY FOR CHEMISTS Paper- V (a2)
Max. Marks	15 (ETE) + 10 (IA) =25

Credit			Total Credits
L	T	P	1
1	0	0	

Course Objectives:
On completion of the course, students are able to:
To introduce structure, function and organization of various bio-molecules present in the living cell.

Course Outcome:
At the end of the course, learners will be able to:
The students will acquire knowledge of molecular structure of proteins, DNA, RNA, carbohydrates, lipids and vitamins, and organization and working principles of various components present in living cell.

Student Learning Outcomes (SLO):
Students will:
1. The chemical basis for biological phenomena and cellular structure.
2. How physiological conditions (esp. the chemistry of water) influence the structures and reactivities of biomolecules.
3. The chemical properties of amino acids, cofactors, and sugar.
4. The basic principles of protein and polysaccharide structure
enzyme kinetics and their application to the elucidation of catalytic mechanisms
constructing reasonable electron-pushing mechanisms for enzyme-catalyzed reactions.
5. How health, disease, and modern medicine are all rooted in biological chemistry

Unit	Syllabus	Periods
UNIT - I	**Cell Structure and Functions** Structure prokaryotic and eukaryotic cells, intracellular organelles and their functions, comparisons of plant and animal cells. Over view of metabolic processes-catabolism and anabolism. ATP the biological energy currency. Origin of life unique properties of carbon chemical evolution and rise of living systems. Introduction to biomolecules, building blocks of bio-macro molecules.	3

UNIT - II	**Carbohydrats** On formation of monosaccharides, structure and functions of important derivatives of monosaccharides like glycosides, deoxy sugars, myoinositol, amino sugars. N-acetyl muramiccid, sialic acid. Disaccharides and polysaccharides: Structural polysaccharides-cellulose and chitin. Storage polysaccharides - starch and glycogen. Structure and biological functions of glucosE amino glycans or mucopolysaccharides. Carbohydrates of glycoproteins and glycolipids. Role of sugars in biological recognition. Blood group substances. Ascorbic acid. Carbohydrate metabolism - Kreb's cycle, glycolysis, glycogenesis and glycogenolysis, gluconeogenesis, pentose phosphate pathway.	3
UNIT - III	**Lipids** Fatty acids, essential fatty acids, structure and function of triacyl glycerols, glycerophospholipids, sphingolipids, cholesterol, bile acids, prostaglandins. Liproproteins- composition and function, role in atherosclerosis. Properties of lipidaggregates-micelles, bilayers, liposomes and their possible biological functions. Biological membranes. Fluid mosaicmodel of membrane structure. Lipid metabolism -β-oxidation of fatty acids.	3
UNIT - IV	**Amino-acids, Peptides and Proteins** Emical and enzymatic hydrolysis of proteins to peptidies, amino acid sequencing. Secondary structure of proteins, for ceresponsible for holding of secondary structures. α- helix, +β-sheets, super secondary structure, triple helix structure of collagen. Tertiary structure of protein-folding and domain structure. Quaternary structure. Amino acid metabolism-degradation and biosynthesis of amino acids, sequence determination: chemical / enzymatic / mass spectral, racemization / detection. Chemistry of oxytocin and tryptophan releasing hormone (TRH).	3
UNIT - V	**NucleicAcids** Purine and pyrimidine bases of nucleic acids, base pairing via H-bonding. Structure of ribonucleic acids (RNA) and deoxyribonucleic acid (DNA), double helix model of DNA and forces responsible for holding it. Chemical and enzymatic hydrolysis of nucleic acids. The chemical basis for heredity, an overview of replication of DNA, transcription, translation and genetic code. Chemical synthesis of mono and trinucleoside.	3

REFERENCE BOOKS –

1 Principles of Biochemistry, A.L. Lehnigher, Worth Publishers.

2 Biochemistry, L. Stryer, W.H. Freeman.

3 Biochemistry, J. David Rawn, Neil Patterson.

4 Biochemistry, Voetand Voet, John Wiley.

5 Outlines of Biochemistry E. E. Connand P.K. Stumpf, John Wiley.

Class	M.Sc. Chemistry (Previuos)
Semester/Year	I Year
Subject & Subject Code	Chemistry - MCHEM20Y107

Paper	English	COMPUTER FOR CHEMISTS Paper- V (b)
	हिन्दी	

Max. Marks	15 (ETE) + 10 (IA) =25

Credit			Total Credits
L	T	P	1
1	0	0	

Course Objectives:

On completion of the course, students are able to:

Provides essential theoretical background of computational chemistry and practical/programming skills to perform scientific computations to solve chemical problems. Students will have exposure on a variety of computational tools in chemical science esp related to research. Gain knowledge about ICH guidelines, i.e., the organization that sets and governs the laws and rules for all the quality tests. Assess the quality of the formulation and assuring the compliance of standards.

Course Outcome:

At the end of the course, learners will be able to:

1. Critically assess the applicability of computational methods to specific problems in chemistry and successfully apply appropriate computational techniques in their academic and scientific careers.
2. Hands on training in the context of currently available computational chemistry software and high-performance computer hardware.

Student Learning Outcomes (SLO):

Students will:

1. Having a clear understanding of the subject related concepts and of contemporary issues.
2. Having computational thinking (Ability to translate vast data in to abstract concepts and to understand database reasoning).
3. Having problem solving ability- solving social issues and engineering problems Should have the patience and determination to learn concepts and apply them.
4. Should be attentive towards details and be accurate towards calculations and observations.
5. Should be a good combination of analytical and scientific skills.
6. Have excellent observation and research skills.
7. Should have problem-solving skills.

Unit	Syllabus	Periods
UNIT - I	**Introduction to computers and Computing** Basic structure and functioning of computer with a PC as an illustrative example. Memory, I/O devices. Secondary storage Computer languages. Operating systems with DOS as an example Introduction to UNIX and WINDOWS. Data processing, principles of programming, Algorithms and flow-charts.	3

UNIT - II	**Computer Programming in FORTRAN / C / BASIC** (the language features are listed here with reference to FORTRAN. The instructormay choose an other language such as BASIC or C the features may be replaced appropriately). Elements of the computer language. Constants and variables. Operations and symbols Expressions. Arithmetic assignment statement. Input and output Format statement.Termination statements. Branching statements such as IF or GO TO statement.	3
UNIT - III	LOGICAL variables Double precession variables. Subscripted variables and DIMENSION. DO statement FUNCTION AND SUBROUTINE. COMMON and DATA statement (Student learn the programming logic and these language feature by hands on experience on a personal computer from the very beginning of this topic.)	3
UNIT - IV	**Programming in Chemistry** Development of small computer codes involving simple formulae in Chemistry, such as Vander Waals equation, pH titration, kinetics, radioactive decay. Evaluation of lattice energy and ionic radii from experimental data. Linear simultaneous equations to solve secular equations with in the Hckel theory.Elementary structural features such as bond lengths, bond angles, dihedral angles, etc. of molecules extracted from a data base such as Cambridge data base.	3
UNIT - V	**Use of Computer programmes** The student will learn how to operate a PC and how to run standard programmes and packages, execution of linear regression, X-Y plot, Numerical Integration and differentiation as well as differential equation solution programmes. Monte Carlo and Moleculuar dynamics, programmes with data preferably from physical chemistry laboratory. Further the student will operate one or two or the packages such as MATLAB, EASYPLOT, LOTUS, FOXPRO and word processing software such as WORD STAR / MS WORD.	3

REFERENCE BOOKS –

1   Fundamentals of Computer: V. Rajaraman (Prentice Hall)

2   Computers in Chemistry: K.V. Raman (Tata Mc Graw Hill)

3   Computer Programming in FORTRAN IV-V Rajaraman (Prentice Hall)

4   Computational Chemistry, A.C. Norris.

Class	M.Sc. Chemistry (Previuos)	
Semester / Year	I Year	
Subject & Subject Code	Practical Chemistry - MCHEM20Y108	
Paper	Paper- I and Paper- II, Practical	
Max. Marks	60 (ETE) + 40 (IA) =100	
Credit	Total Credits	

L	T	P	4
0	0	4	

PRACTICALS

Inorganic Chemistry

Qualitative and Quantitative Analysis

1. Less common metal ions : Tl, Mo, W, Ti, Zr, Th, V, U (two metal ions in cationic / anionic forms).

2. Insolubles: Oxides, sulphates and halides.

3. Separation and determination of two metal ions Cu-Ni, Ni-Zn, Cu-Fe etc. involving volumetric and gravimetric methods.

Chromatography

Separation of cations and anions by

a. Paper Chromatography.
b. Column Chromatography: Ion exchange.

Preparations

Preparation of selected in organic compounds and their studies by I.R. electronic spectra, Mssbauer, E.S.R. and magnetic susceptibility measurements. Handling of air and moisture sensitive compounds.

1. $VO\,(acac)_2$
2. $TiO\,(C_9H_8NO)_2 2H_2O$
3. cis-$K\,[Cr\,(C_2O_4)_2(H_2O)_2]$
4. $Na[Cr(NH_3)_2(SCN)_4]$
5. $Mn\,(acac)_3$
6. $K_3\,[Fe(C_2O_4)_3]$
7. Prussian Blue, Turnbull's Blue.
8. $[Co(NH_3)_6]\,[Co(NO_2)_6]$
9. cis-$[Co(trien)\,(NO_2)_2]Cl.H_2O$
10. $Hg[Co(SCN)_4]$
11. $[Co(Py)_2Cl_2]$
12. $[Ni(NH_3)_6]Cl_2$
13. $Ni(dmg)_2$
14. $[Cu(NH_3)_4]\,SO_4 H_2O$

PRACTICAL

Organic Chemistry

Qualitative Analysis

Separation, purification and identification of compounds of binary mixture (one liquid and one solid) using T and columns chromatography, chemical tests. IR spectra to be used for functional group identification.

Organic Synthesis

Acetylation : Acetylation of cholesterol and sepration of cholesteryl acetate by columncl

Oxidation: Adipic acid by chromic acid oxidation of cyclohexanol.
Grignard reaction: Synthesis of triphenyl methanol from benzoic acid.
Aldol condensation: Dibenzal acetone from benzaldehyde.
Sandmeyer reaction: p-Chlorotoluene from p-toluidine.
Acetoacetic ester Condensation : Synthesis of ethyl-n-butylacetoacetate by A.E.E. condensation.
Cannizzaro reaction: 4-Chlorobenzaldehyde as substrate.
Friedel Crafts reaction : β-Benzoyl propionic acid from succinic anhydride and benzene.
Aromatic electrophilic sustitutions: Synthesis of p-nitro aniline and p-bromoaniline.
The Products may be Characterized by Spectral Techniques.

Quantitative Analysis

Determination of the percentage or number of hydroxyl groups in an organic compound by acetylation method.
Estimation of amines/ phenols using bromate bromide solution/ or acetylation method.Determination of Iodine and Saponification values of an oil sample.
Determination of DO, COD and BOD of water sample.

Class	M.Sc. Chemistry (Previuos)		
Semester / Year	I Year		
Subject & Subject Code	Practical Chemistry - MCHEM20Y109		
Paper	Paper- III, Practical		
Max. Marks	60 (ETE) + 40 (IA) =100		
Credit	Total Credits		
L	T	P	4
0	0	4	

PRACTICAL

Physical Chemistry

Error Analysis and Statistical Data Analysis

Errors, types of errors, minimization of errors distribution curves precision, accuracy and combination; statistical treatment for error analysis, student 't test, null hypothesis, rejection criteria, F&Q test; linear regression analysis, curve fitting. Calibration of volumetric apparatus, burette, pipette and standard flask.

Adsorption

To study surface tension-concentration relationship for solutions (Gibbs equation).

PhaseEquilibria

i. Determination of congruent composition and temperature of a binary system (e.g.diphenyl amine-benzophenone system).

ii. Determination of transition temperature of given salt (e.g., $CaCl_2$) conductometrically.

iii. To construct the phase diagram for three component system(e.g.chloroform-acetic acid-water).

Chemical Kinetics

Determination of the effect of (a) Change of temperature (b) Change of concentration of reactant and catalyst and(c)Ionic strength of the media on the velocity constant of hydrolysis of an ester / ionic reaction.

i. Determination of the velocity constant of hydrolysis of anester / ionic reaction in micellar media.

ii. Determination of the velocity constant for the oxidation of iodide ions by hydrogen peroxide studing the kinetics as an iodine clock reactions.

iii. Flowing clock reactions (Ref: Experiments in Physical Chemistry by Show maker)

iv. Determination of the primary salt effect on the kinetics of ionic reaction and testing of the Bronsted relationship (iodide ionis oxidised by persulphateion).

v. Oscillatory reaction.

Solution

1 Determination of molecular weight of non-volatile and non-electrolyte / electrolyte by cryoscopic method and to determine the activity coefficient of an electrolyte.

2 Determination of the degree of dissociation of weak electrolyte and to study the deviation from ideal behavior that occurs with a strong electrolyte.